INSTITUT NATIONAL DE RECHERCHE EN INFORMATIQUE ET EN AUTOMATIQUE

A Positive MUSCL Scheme for Triangulations

Paul-Henry Cournède, Christophe Debiez, Alain Dervieux

N° 3465

Juillet 1998

THÈME 4

Rapport de recherche

ISSN 0249-6399

A Positive MUSCL Scheme for Triangulations

Paul-Henry Cournède, Christophe Debiez, Alain Dervieux

Thème 4 — Simulation et optimisation
de systèmes complexes
Projet SINUS

Rapport de recherche n° 3465 — Juillet 1998 — 19 pages

Abstract: In this paper, we link together and extend some results that have previously been given about positive schemes in the approximation of compressible flows. We mainly turn here to bidimensional problems and spatially high-order schemes (at least second-order) of MUSCL type, defined on unstructured triangulations, for an explcit time discretization. In the case of the scalar advection equation, we derive a scheme preserving the positivity of the advected quantity. Moreover, if the advection velocity is divergence free, our scheme is LED. Then, we manage to preserve the positivity of density when solving the Euler equations and, in the multi-component case, we also preserve the maximum principle for mass fractions.

Key-words: finite-volume methods, triangulation, MUSCL, positive and LED schemes, maximum principle

* Laboratoire de Mathématiques Appliquées aux Systèmes, Ecole Centrale Paris, 92 295 Châtenay Malabry Cédex, FRANCE
† INRIA Sophia-Antipolis, B.P. 93, 2004 Route des Lucioles, 06902 Sophia-Antipolis Cédex, FRANCE
‡ INRIA Sophia-Antipolis, B.P. 93, 2004 Route des Lucioles, 06902 Sophia-Antipolis Cédex, FRANCE

Un Schéma MUSCL positif pour les maillages triangulaires

Résumé : Dans ce rapport, nous nous intéressons à la construction de schémas positifs pour la résolution numérique des équations d'Euler, plus particulièrement pour des problèmes bidimensionnels sur maillages triangulaires. Nous proposons ainsi un schéma de type MUSCL du troisième ordre (quasiment) qui préserve la positivité de la masse volumique et qui préserve le principe du maximum pour les fractions massiques lors d'écoulements multi-espèces.

Mots-clés : Méthode volumes finis, maillage triangulaire, MUSCL, schémas positifs et LED, principe du maximum

1 Introduction

Unstructured-mesh numerical methods are easily and quickly applied to various types of problem, which makes them highly interesting for CFD engineers. A crucial point in the development of these methods is robustness, which is mainly related to their abilities to provide solutions that keep positive several physical quantities: pressure, density, temperature, mass fractions, turbulent kinetic energy and dissipation rate, etc.

For the 1D scalar advection equation, a positive first-order accurate approximation can be built by applying some upwinding principles such as the Godunov method, but it is usually not accurate enough. This first-order scheme can be extended to high-order ones by introducing limiters which can be chosen to preserve positivity or TVD properties.

Among the different ways to introduce limiters, the MUSCL method (Monotonic Upwind scheme for Conservation Laws) introduced by Van Leer in [17] is particularly attractive. It is based on the application of the Godunov method to flow values that result of cell-wise higher-order interpolation. The advantage of MUSCL is its modularity, and e.g. the possibility of improving the accuracy of the scheme by improving the cell reconstruction.

In the case of 2D (or 3D) schemes, TVD-like properties do not readily generalize, especially for unstructured meshes, but some positivity results were obtained by Barth in [2] by using multidimensional reconstruction and limitation. A different strategy is the element-wise limitation introduced in MDHR (Multi-Dimensional High Resolution) approximation, cf. Sidilkover in [16] and Deconinck *et al.* in [6], it also leads to positivity results. Concerning methods involving edgewise interpolation and limitation, a notable contribution was brought by Jameson in [11]. He proposed a LED (Local Extremum Diminishing) scheme based on a special molecule often referred to as the "upwind-triangle edge fluxes" [SFPD].

The Jameson scheme is of symmetric-TVD type, which means that for each flux, a unique limiter decides of the convenient combination of two (symmetric) schemes.

In this paper, we restrict ourselves to an explicit time discretization and we study a genuinely MUSCL version of the Jameson scheme: the interpolation limitation is realized thanks to the so-called upwind triangle, and an extra interpolation may give the high-order asymptotic accuracy (i.e. far from extrema). For the scalar advection equation, this scheme is positive.

An important application of limiters is the Euler equations, for which neither TVD nor LED statements hold. However, there exist several schemes that are known to preserve the positivity of density and temperature in 1D for an explicit discretization, under an appropriate CFL condition. The first one is the Godunov scheme, based on the exact solution of the Riemann Problem. The HLLE scheme was then derived, as a positive correction of the Roe's scheme, cf. [7]. The last one that we shall present is a flux-splitting scheme developed by Perthame in [14].

An important issue is to examine whether these schemes can be adapted to bidimensional problems and to a higher-order of accuracy with our limiters, whilst still preserving the positivity of density.

Another issue concerns the behavior of passive species for example in multi-component flows or turbulence models. In both cases, positivity and even preservation of the maximum principle for the mass fractions or k and ϵ are crucial for robustness.

In the case of multi-component flows, Larrouturou derived in [13] a second-order 1D scheme and a first-order 2D (and 3D) scheme that preserve the maximum principle. Concerning the closure variables k and ϵ of the well-known turbulence model, Jongen *et al.* discussed the design of 1D and 2D positive schemes on structured meshes, cf. [12].

The third focus of this paper is to use our limiters to derive a high-order bidimensional scheme on unstructured meshes that still preserves the maximum principle for the passive variables, starting from Larrouturou's approach.

The report is consequently organized as follows: firstly in Section 2, the scalar advection equation is considered and allows us to introduce the main features of the scheme. In Section 3, we apply the introduced methodology to the 2D Euler equations, and finally, Section 4 is devoted to the maximum principle for passive species.

2 Positive Schemes - LED Schemes for the Scalar Advection Equation

2.1 Positive Schemes - LED Schemes

In this section we consider a scalar time dependent conservation equation on an arbitrary (possibly unstructured) grid:

$$U_t + F_x(U) + G_y(U) = 0 \tag{1}$$

Assuming that the mesh points are numbered, we call U_i the value at mesh point i.

Lemma 1 : A positivity criterion
Suppose that the semi-discrete approximation of equation (1) can be expressed in the form:

$$\frac{dU_i}{dt} = L(U) = b_i U_i + \sum_{j\neq i} b_j U_j \ , \tag{2}$$

where all the b_j, $j \neq i$, are non-negative and $b_i \in \Re$. Then the corresponding explicit first-order scheme preserves positivity under an appropriate CFL-like condition.

The proof is straightforward. The complete explicit first-order discretization can be written as:

$$\frac{U_i^{n+1} - U_i^n}{\Delta t} = L(U^n) = b_i U_i^n + \sum_{j\neq i} b_j U_j^n \ ,$$

that is to say:

$$U_i^{n+1} = (1 + \Delta t b_i) U_i^n + \sum_{j\neq i} (\Delta t \ b_j) U_j^n \ ,$$

Therefore, if $b_i \geq \frac{1}{\Delta t}$ (the CFL-like condition), all the coefficients are non-negative and the scheme preserves positivity: if at time n all the U_i are positive, so will be U_i^{n+1}. □

Remark 1 *Under a perhaps different restriction on Δt, a high-order explicit time discretization can still preserve positivity.*

The idea dates back to the works of Shu, cf. [15]. A general high-order explicit time discretization can be written in the form:

$$\left\{ \begin{array}{rcl} U_i^{(0)} & = & U_i^n \\ U_i^{(j)} & = & \sum_{k=0}^{j-1} \left(\alpha_{jk} U_i^{(k)} + \Delta t \, \beta_{jk} L(U^{(k)}) \right) \quad j = 1, \ldots, m \\ U_i^{(m)} & = & U^{n+1} \end{array} \right.$$

with $\sum_k \alpha_{jk} = 1$ for consistency.

If all the coefficients α_{jk} and β_{jk} are non-negative, $U^{(j)}$ is a convex combination of terms in the form:

$$U_i^{(k)} + \Delta t \ \frac{\beta_{jk}}{\alpha_{jk}} \ L(U^{(k)})$$

They correspond to first-order time discretizations with time steps equal to $\left(\Delta t\,\frac{\beta_{jk}}{\alpha_{jk}}\right)$ and thus are positive provided that:

$$b_i\,\Delta t\,\frac{\beta_{jk}}{\alpha_{jk}} \geq 1 \text{ for all } j \text{ and } k\ .$$

In particular, we recall here the third-order time discretization given in [15]:

$$\left\{\begin{array}{rcl} U_i^{(1)} & = & U_i^n + \Delta t\, L(U^n) \\ U_i^{(2)} & = & \frac{3}{4}U_i^n + \frac{1}{4}U_i^{(1)} + \frac{1}{4}\Delta t\, L(U^{(1)}) \\ U_i^{n+1} & = & \frac{1}{3}U_i^n + \frac{2}{3}U_i^{(2)} + \frac{2}{3}\Delta t\, L(U^{(2)}) \end{array}\right.$$

We have $\min_{j,k}\frac{\beta_{jk}}{\alpha_{jk}} = 1$ and the CFL condition to preserve positivity for this third-order time discretization is the same as for the first-order one. □

We recall now the theory introduced by Jameson in [11] on Local Extremum Diminishing (LED) schemes.

Lemma 2 : A LED criterion
If the semi-discretization of Equation (1) can be written in the form:

$$\frac{dU_i}{dt} = \sum_{k\in V(i)} c_{ki}(U)\,(U_k - U_i)\,. \tag{3}$$

with all the $c_{ki}(U) \geq 0$, then a local maximum can not increase, and a local minimum can not decrease.

Proof: If U_i is a local maximum, then for all $k \in V(i)$, ($V(i)$ contains the neighbours of node i), $(U_k - U_i) \leq 0$, and thus $\frac{dU_i}{dt} \leq 0$, the local maximum will not increase, nor a local minimum decrease. □
Such a scheme will be called a **Local Extremum Diminishing** (LED) scheme. It preserves positivity.

In the sequel, we will consider the following scalar conservative equation for a bidimensional problem:

$$U_t + div(\vec{V}\,U) = 0\ , \tag{4}$$

where $\vec{V}$ is a given advection velocity in $\mathbb{R}^2$.

2.2 First-Order Positive Scheme

We use a vertex-centred finite-volume approximation. The cells are delimited by the **triangle medians**, cf. Figure 1.

General semi-discretizations of Equation (4) are those of Baba-Tabata, cf. [1], which can be written as:

- a centred scheme:

$$a_i\,\frac{dU_i}{dt} + \sum_{j\in V(i)} \vec{V_{ij}}.\vec{\eta_{ij}}\,(\frac{U_i + U_j}{2}) = 0$$

where a_i is the area of cell C_i, $V(i)$ contains the neighbours of node i, $\vec{V_{ij}}$ is the approximated value of the advection velocity at the interface between cells i and j, and $\vec{\eta_{ij}} = \int_{\partial C_i \cap \partial C_j} \vec{n}\,d\sigma$.

- an upwind scheme:

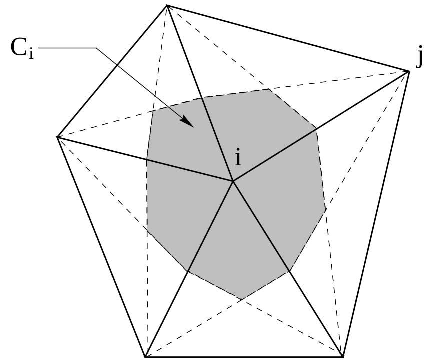

Figure 1: The control volume C_i

$$a_i \frac{dU_i}{dt} + \sum_{j\in V(i)} \vec{V_{ij}}.\vec{\eta}_{ij} \begin{cases} U_i & \text{si } \vec{V_{ij}}.\vec{\eta}_{ij} \geq 0 \\ U_j & \text{si } \vec{V_{ij}}.\vec{\eta}_{ij} \leq 0 \end{cases} = 0\,. \tag{5}$$

If we use the well-known notations:

$$a^+ = \frac{a+|a|}{2} \quad and \quad a^- = \frac{a-|a|}{2} \quad a \in \Re\,,$$

Equation (5) can also be written:

$$a_i \frac{dU_i}{dt} = -\sum_{j\in V(i)} (\vec{V_{ij}}.\vec{\eta}_{ij})^+ U_i - \sum_{j\in V(i)} (\vec{V_{ij}}.\vec{\eta}_{ij})^- U_j \tag{6}$$

or:

$$a_i \frac{dU_i}{dt} + \underbrace{\sum_{j\in V(i)} \vec{V_{ij}}.\vec{\eta}_{ij} (\frac{U_i + U_j}{2})}_{\text{centred}} + \underbrace{\sum_{j\in V(i)} \frac{1}{2} |\vec{V_{ij}}.\vec{\eta}_{ij}| (U_i - U_j)}_{\text{upwind}} = 0\,. \tag{7}$$

Considering the semi-discretization (6), we have:

$$\frac{dU_i}{dt} = \left(-\frac{1}{a_i} \sum_{j\in V(i)} (\vec{V_{ij}}.\vec{\eta}_{ij})^+\right) U_i + \sum_{j\in V(i)} \underbrace{\left(-\frac{1}{a_i}(\vec{V_{ij}}.\vec{\eta}_{ij})^-\right)}_{\geq 0} U_j$$

It is exactly the required form to preserve positivity, using Lemma 1 in Section 2.1, and we have shown the following lemma:

Lemma 3 *The upwind scheme (6) is positive under the CFL condition:*

$$\frac{\Delta t}{a_i} \sum_{j\in V(i)} (\vec{V_{ij}}.\vec{\eta}_{ij})^+ \leq 1$$

Remark 2 *If the advection velocity is divergence free, in particular uniform, this upwind scheme is LED.*

As a matter of fact we can write:

$$\sum_{j\in V(i)} (\vec{V_{ij}}.\vec{\eta}_{ij}) U_i = 0 \tag{8}$$

It is straightforward if $\vec{V}$ is uniform, because $\sum_{j\in V(i)} \vec{\eta}_{ij} = 0$, and if $div(\vec{V}) = 0$, integrating over cell i and using the Stokes formula, we get:

$$\oint_{\delta C_i} \vec{V}.\vec{\eta} = 0\,,$$

which gives after discretization:

$$\sum_{j\in V(i)} (\vec{V_{ij}}.\vec{\eta}_{ij}) = 0 \tag{9}$$

and it leads to (8) again.
It allows us to rewrite (6) as follows:

$$\frac{dU_i}{dt} = \sum_{j\in V(i)} \underbrace{\Big(-\frac{1}{a_i}(\vec{V_{ij}}.\vec{\eta}_{ij})^-\Big)}_{\geq 0}(U_j - U_i) \tag{10}$$

Using the Jameson lemma of Section 1, the scheme is LED.

2.3 Limited High-Order Schemes

Higher-order schemes are obtained by a better interpolation in the cells. The flux function ϕ_{ij} at the interface between cells i and j was $\phi_{ij} = \phi(U_i, U_j)$ for the first order, it is now evaluated using better left and right values at the interface, $\phi_{ij} = \phi(U_{ij}, U_{ji})$, where U_{ij} and U_{ji} are interpolation results:

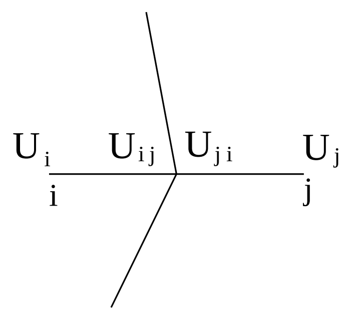

Figure 2: Interface values

But, to keep the scheme non oscillatory and positive, we introduce **flux limiters**. The idea dates back to the works of Boris and Book in [3].
In the case of unstructured meshes, second-order positive schemes were derived using two-entry symmetric limiters by Jameson in [11] and MUSCL formulations were introduced by Debiez *et al.* in [4] and [5].
We examine here the upwind schemes proposed by Debiez *et al.* in [5] using three-entry limiters, which allows us to design a positive scheme, of third or fifth order far from extrema, when U is smoothly varying.

The semi-discretization of:

$$U_t + div(\vec{V}\ U) = 0\ , \tag{11}$$

is now written:

$$a_i\,\frac{dU_i}{dt} = -\sum_{j\in V(i)} (\,\vec{V_{ij}}.\vec{\eta}_{ij}\,)^+\,(U_i + \frac{1}{2}L_{ij}(U)) \;-\; \sum_{j\in V(i)} (\,\vec{V_{ij}}.\vec{\eta}_{ij}\,)^-\,(U_j + \frac{1}{2}L_{ji}(U))\,. \tag{12}$$

To define $L_{ij}(U)$ and $L_{ji}(U)$ we use the downstream and upstream triangles T_{ij} and T_{ji}, cf. Figure 3, as introduced by Dervieux and Fezoui in [9], and we define:

$$\Delta^- U_{ij} \;=\; \vec{\nabla} U\,|_{T_{ij}}\,.\,\vec{ij} \qquad \Delta^0 U_{ij} = U_j - U_i \qquad \Delta U_{ji} \;=\; \vec{\nabla} U\,|_{T_{ji}}\,.\,\vec{ij}\,,$$

where the gradients are those of the discretized function U.

Jameson has given the following interesting property in [11]:

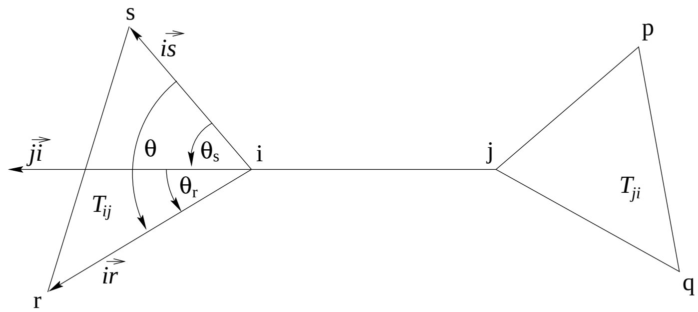

Figure 3: Downstream and Upstream Triangles

Lemma 4 *We can write:*

$$\Delta^{-} U_{ij} \;=\; \epsilon_{si}\,(U_i \;-\; U_s) \;+\; \epsilon_{ri}\,(U_i \;-\; U_r)\,,$$

and

$$\Delta^{-} U_{ji} \;=\; \epsilon_{jp}\,(U_p \;-\; U_j) \;+\; \epsilon_{jq}\,(U_q \;-\; U_j)\,,$$

where the coefficients ϵ_{si}, ϵ_{ri}, ϵ_{jp} and ϵ_{jq} are all positive (possibly zero).

Proof: A short calculation gives:

$$\vec{ji} = \epsilon_{si}\;\vec{is} \;+\; \epsilon_{ri}\;\vec{ir}$$

with:

$$\left\{\begin{array}{lcl} \epsilon_{si} & = & \dfrac{l_j}{l_s}\,\left(\dfrac{\sin\theta_r}{\sin\theta}\right) \\[2ex] \epsilon_{ri} & = & \dfrac{l_j}{l_r}\,\left(\dfrac{\sin\theta_s}{\sin\theta}\right) \end{array}\right.$$

with $l_j = ||\vec{ij}||$, $l_r = ||\vec{ir}||$ and $l_s = ||\vec{is}||$.
ϵ_{ri} and ϵ_{si} are both positive.

$$\vec{\nabla} U\,|_{T_{ij}}\,.\,\vec{ij} = \vec{\nabla} U\,|_{T_{ij}}\,.\,(\epsilon_{si}\,\vec{si} \;+\; \epsilon_{ri}\,\vec{ri})$$

As the discretized function U is linear in every triangle, we get:

$$\left\{\begin{array}{lcl} \vec{\nabla} U\,|_{T_{ij}}\,.\,\vec{si} & = & U_i - U_s \\[2ex] \vec{\nabla} U\,|_{T_{ij}}\,.\,\vec{ri} & = & U_i - U_r \end{array}\right.$$

Thus:

$$\Delta^{-} U_{ij} \;=\; \epsilon_{si}\,(U_i \;-\; U_s) \;+\; \epsilon_{ri}\,(U_i \;-\; U_r)\;,$$

with ϵ_{si} and ϵ_{ri} positive. □

Now, we introduce a family of limiters with three entries, satisfying:

$(P1)$ $L(u,v,w) \;=\; L(v,u,w)$

$(P2)$ $L(\alpha\,u, \alpha\,v, \alpha\,w) \;=\; \alpha\,L(v,u,w)$

$(P3)$ $L(u,u,u) \;=\; u$

$(P4)$ $L(u,v,w) \;=\; 0$ if $uv \leq 0$

and we are going to use the following one:

$$\left\{ \begin{array}{lcl} L(u,v,w) & = & 0 \qquad \text{si} \quad uv \leq 0 \\ \\ & = & Sign(u)\ \min(\,2\,|u|\,,\,2\,|v|\,,\,|w|) \quad \text{otherwise} \end{array} \right. \tag{13}$$

We take $L_{ij}(U) = L(\Delta^- U_{ij}\,,\,\Delta^0 U_{ij}\,,\,\Delta^{HO} U_{ij})$ and $L_{ji}(U) = L(\Delta^- U_{ji}\,,\,\Delta^0 U_{ji}\,,\,\Delta^{HO} U_{ji})$.
When $L_{ij}(U) = 0$, we switch to the first-order scheme of Baba-Tabata and when the limitation is not active, $L_{ij}(U) = \Delta^{HO} U_{ij}$, the scheme is of high order.
We take for example:

$$\Delta^{HO} U_{ij} = \frac{1}{3}\,\Delta^- U_{ij} + \frac{2}{3}\,\Delta^0 U_{ij}\,, \tag{14}$$

which gives us a third-order scheme.

Lemma 5 *This scheme is positive under an appropriate CFL condition.*

Proof: First, we can note that:

$$L_{ij}(U) = K^- \Delta^- U_{ij} = K_1^0 \Delta^0 U_{ij}$$

where K^- and K_1^0 are positive. Likewise, we get that:

$$L_{ji}(U) = K_2^0 \Delta^0 U_{ji} = -K_2^0 \Delta^0 U_{ij}$$

where K_2^0 is positive. We can thus rewrite the semi-discretized Equation (12) in the following form:

$$a_i \frac{dU_i}{dt} = - \sum_{j \in V(i)} (\vec{V_{ij}}.\vec{\eta}_{ij})^+ (U_i + \frac{1}{2} K^- \Delta^- U_{ij}) \;-\; \sum_{j \in V(i)} (\vec{V_{ij}}.\vec{\eta}_{ij})^- (U_j - \frac{1}{2} K_2^0 \Delta^0 U_{ij})$$

that is to say:

$$\begin{array}{rcl} a_i \dfrac{dU_i}{dt} & = & - \displaystyle\sum_{j \in V(i)} (\vec{V_{ij}}.\vec{\eta}_{ij})^+ \Big(U_i + \frac{1}{2} K^- \Big(\epsilon_{si}(U_i - U_s) + \epsilon_{ri}(U_i - U_r) \Big) \Big) \\ & & - \displaystyle\sum_{j \in V(i)} (\vec{V_{ij}}.\vec{\eta}_{ij})^- \Big(U_j - \frac{1}{2} K_2^0 (U_j - U_i) \Big) \end{array}$$

which can thus be written:

$$a_i \frac{dU_i}{dt} = \alpha_i U_i + \sum_{k \in V(i)} \alpha_k U_k + \sum_{j \in V(i)} \beta_j (1 - \frac{K_2^0}{2}) U_j \tag{15}$$

where all the α_k and β_j are positive, and α_i is positive or negative. According to Lemma 1, this form corresponds to a positive scheme, provided that $K_2^0 \leq 2$. This condition is satisfied for the proposed scheme, which ends the proof. □

Remark 3

Let us examine a bit further the CFL condition needed to ensure positivity. In Equation (15),

$$\alpha_i = - \sum_{j \in V(i)} (\vec{V_{ij}}.\vec{\eta}_{ij})^+ \Big(1 + K^- \frac{(\epsilon_{si} + \epsilon_{ri})}{2} \Big) + \sum_{j \in V(i)} \Big(-(\vec{V_{ij}}.\vec{\eta}_{ij})^- \Big) \frac{K_2^0}{2}$$

The explicit discretization gives the following condition for positivity:

$$\frac{\Delta t}{a_i} \sum_{j \in V(i)} (\vec{V_{ij}}.\vec{\eta}_{ij})^+ \Big(1 + K^- \frac{(\epsilon_{si} + \epsilon_{ri})}{2} \Big) \leq 1$$

A mesh-depending quantity is involved here:

$$M_{ij} = (\epsilon_{si} + \epsilon_{ri}) = \frac{l_j^2}{l_s l_r}\left(\frac{l_r \sin\theta_r + l_s \sin\theta_s}{l_j \sin\theta}\right).$$

For cartesian orthogonal meshes, M_{ij} is uniformly equal to 1, but it can be very big, and thus very penalizing, for very irregular meshes. Let us denote $M = \max_{i,j} M_{ij}$, let us introduce $|V_{max}|$, the maximum value of the advection velocity.
As $K_2^0 \leq 2$, the CFL condition to ensure positivity can be written:

$$\frac{|V_{max}|\ \Delta t}{a_i} \sum_{j\in V(i)} l_{ij} \leq \frac{1}{1+M}\ ,$$

where $l_{ij} = ||\vec{\eta_{ij}}|| = ||\int_{C_i \cap C_j} \vec{\eta}\ ds\ ||$.
Let us introduce $L_i = \sum_{j\in V(i)} l_{ij}$, which plays the role of a cell-boundary measure and we finally get:

$$\frac{|V_{max}|\ \Delta t}{(\frac{a_i}{L_i})} \leq \frac{1}{1+M}\ . \tag{16}$$

For this CFL condition to be acceptable, we need to have a control on the regularity of the mesh. In particular, M has to be bounded for the mesh family considered for the asymptotic convergence.

Remark 4 *If the advection velocity is divergence free (in particular uniform), the scheme is LED.*

We are just going to give a sketch of the proof, which is close to the one given for the first-order scheme. We add in the right hand side of the semi-discretized Equation (12) the nil term $\sum_{j\in V(i)}(\vec{V_{ij}}.\vec{\eta_{ij}})\, U_i$, which gives:

$$a_i \frac{dU_i}{dt} = -\sum_{j\in V(i)} (\vec{V_{ij}}.\vec{\eta_{ij}})^+ \frac{1}{2} L_{ij}(U) - \sum_{j\in V(i)} (\vec{V_{ij}}.\vec{\eta_{ij}})^- \Big((U_j - U_i) + \frac{1}{2} L_{ji}(U)\Big)$$

And replacing the limited corrections by their expressions in terms of differences $(U_k - U_i)$ as we did before, we get:

$$a_i \frac{dU_i}{dt} = \sum_{k\in V(i)} \gamma_k (U_k - U_i) + \sum_{j\in V(i)} \delta_j (1 - \frac{K_2^0}{2})(U_j - U_i)$$

where all the γ_k and δ_j are positive, and as $K_2^0 \leq 2$, the scheme is LED by Jameson's lemma. □

Remark 5

For U smooth enough, assuming that the mesh size is smaller than α (small), there exist $\epsilon(\alpha)$ such that:
if $\dfrac{|\vec{\nabla} U.\vec{ij}|}{||\vec{ij}||} > \epsilon(\alpha)$ on a segment ij, then the limiter L_{ij} is not active, $L_{ij}(U) = \Delta^{HO} U_{ij}$.

Some examples of higher-order schemes are given by Debiez *et al.* in [4].

3 Positive Schemes for the Euler Equations

In the second part of this paper, we turn to the Euler equations, the robustness of a numerical scheme will highly depend on its capacity to preserve positive density and temperature. We shall give results for the density.
After a short recall of some classical 1D positive schemes, we will derive a 2D-CFL condition ensuring that the 2D schemes corresponding to these 1D positive schemes still preserve the positivity of ρ.

3.1 The Euler Equations

We first recall the conservative form of the Euler Equations in one dimension:

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} = 0 \tag{17}$$

$$U = \begin{pmatrix} \rho \\ \rho u \\ e \end{pmatrix} \qquad F(U) = \begin{pmatrix} \rho u \\ \rho u^2 + P \\ (e+P)u \end{pmatrix} \tag{18}$$

Here u is the velocity and e the total energy per unit area, $e = \rho\epsilon + \frac{1}{2}\rho(u^2 + v^2)$, where ϵ is the internal energy per unit mass. For an ideal gas, the pressure P is defined through an equation of state of the form:

$$P = (\gamma - 1)\epsilon\rho \ .$$

The general form of an explicit conservative scheme for the Euler Equations is:

$$U_i^{n+1} = U_i^n - \frac{\Delta t}{\Delta x}(F_{i+1/2}^n - F_{i-1/2}^n) \ , \tag{19}$$

where U_i^n is the average on the mesh $(x_{i-1/2} \ , \ x_{i+1/2})$.
We will denote $\sigma = \frac{\Delta t}{\Delta x}$.

3.2 Godunov's Method

We solve two independent Riemann problem at each cell interfaces, that do not interact in the cell, provided that:

$$\frac{|\lambda_{max}| \ \Delta t}{\Delta x} < \frac{1}{2} \ ,$$

where $|\lambda_{max}|$ denotes the maximum absolute value of the Riemann Problem wave speeds. We obtain U_i^{n+1} by averaging:

$$U_i^{n+1} = \frac{1}{\Delta x}\int_0^{\frac{\Delta x}{2}} W_{RP}(\frac{x}{\Delta t}, i-1/2) \ dx \ + \ \frac{1}{\Delta x}\int_{-\frac{\Delta x}{2}}^{0} W_{RP}(\frac{x}{\Delta t}, i+1/2) \ dx \ ,$$

where W_{RP} is the exact solution of the Riemann Problem.
We define the set of admissible states E, it contains all the states with a positive density and a positive internal energy. We can write:

$$E = \left\{ U \ \ such \ \ that \ \ \rho > 0 \ \ and \ \ \rho\epsilon = e - \frac{1}{2}\rho u^2 > 0 \right\}$$

E is a convex set, and the Godunov method evaluates U_i^{n+1} as a convex averaging of the Riemann Problem solutions, which is a convex function of the states U_j^n (as long as no vacuum appears). Therefore, if the U_j^n are in E, so is U_i^{n+1}.

Lemma 6 *Under the CFL condition:*

$$\frac{|\lambda_{max}| \ \Delta t}{\Delta x} < \frac{1}{2} \ ,$$

the Godunov scheme preserves the positivity of density and temperature.

3.3 The HLLE Scheme

Since solving the Riemann Problem is expensive, many schemes use an approximate solution to the Riemann Problem, based on the resolution of the linearized Euler equations. But these methods can yield negative density or energy in some cases, cf. Einfeldt in [8].
Using an idea introduced by Harten, Lax and Van-Leer in [10], Einfeldt developed an approximate Riemann Solver that leads to a conservative positive scheme, cf. [8]. It consists of three constant states:

$$W_{HLLE}(\frac{x}{t}, i+1/2) = \begin{cases} U^i & for \;\; \frac{x}{t} < b^l_{i+1/2} \\ \\ U^{i+1/2} & for \;\; b^l_{i+1/2} < \frac{x}{t} < b^r_{i+1/2} \\ \\ Ui+1 & for \;\; b^r_{i=1/2} < \frac{x}{t} \end{cases}$$

where the average state $U^{i+1/2}$ is such that the Riemann Solver is consistant with the integral form of the conservation law, and where $b^r_{i+1/2}$ and $b^l_{j+1/2}$ are numerical approximation for the largest and smallest physical signal-velocities of the exact solution to the Riemann Problem:

$$\begin{cases} b^l_{i+1/2} & = & \min\{a^1_{i+1/2}, u_i - c_i\} \\ b^r_{i+1/2} & = & \max\{a^3_{i+1/2}, u_{i+1} + c_{i+1}\} \end{cases}$$

where $a^k_{i+1/2}$, $k = 1, 2, 3$ are the eigenvalues of the Roe linearization of the Euler equations and $c = \left(\frac{\gamma P}{\rho}\right)^{1/2}$ is the sound speed.
If:

$$\frac{max(|b^l_{i+1/2}|, |b^r_{i-1/2}|)\ \Delta t}{\Delta x} < \frac{1}{2} \ ,$$

the problems at interfaces $i - 1/2$ et $i + 1/2$ do not interact, and we also get that:

$$U^n_{i+1/2} = \frac{1}{(b^r_{i+1/2} - b^l_{i+1/2})\ \Delta t} \quad \int_{b^l_{i+1/2}\Delta t}^{b^r_{i+1/2}\Delta t} \quad W_{RP}(\frac{x}{\Delta t}, i+1/2)\ dx \ ,$$

that is to say a convex function of the states U^n_j. Therefore, we can comclude that if the U^n_j are in E, the set of admissible states, so is U^{n+1}_i.

Lemma 7 *Under the CFL condition*

$$\frac{max(|b^l_{i+1/2}|, |b^r_{i-1/2}|)\ \Delta t}{\Delta x} < \frac{1}{2} \ ,$$

the HLLE scheme preserves the positivity of density and temperature.

3.4 A Kinetic Scheme

Perthame introduced a kinetic scheme preserving the positivity of ρ and T.
First, we semi-discretize the scalar transport equations:

$$\begin{cases} \dfrac{\partial \phi}{\partial t} + \dfrac{\partial (v\phi)}{\partial x} = 0 \\ \\ \dfrac{\partial \psi}{\partial t} + \dfrac{\partial (v\psi)}{\partial x} = 0 \end{cases}$$

We obtain:

$$\begin{array}{ll} \phi^{n+1}_i(v) - \phi^n_i(v) + \sigma[(v^+\phi^n_i(v) + v^-\phi^n_{i+1}) - (v^+\phi^n_{i-1}(v) + v^-\phi^n_i)] & = 0 \\ \psi^{n+1}_i(v) - \psi^n_i(v) + \sigma[(v^+\psi^n_i(v) + v^-\psi^n_{i+1}) - (v^+\psi^n_{i-1}(v) + v^-\psi^n_i)] & = 0 \end{array}$$

Perthame gives us two even non-negative functions χ and ζ such that:

$$\int_{\Re}(1,w^2)\chi(w)\ dw=(1,1) \qquad \text{and} \qquad \int_{\Re}\zeta(w)\ dw=\frac{1}{(\gamma-1)}\ ,$$

with a positive constant β such that $\chi(w)$ and $\zeta(w)$ are non zero only for $|w|\le\sqrt{\beta}$.
These consistency relations combined with the following formulations for the transport functions:

$$\phi_i^n(v)=\frac{\rho_i^n}{\sqrt{T_i^n}}\ \chi\Big(\frac{(v-u_i^n)}{\sqrt{T_i^n}}\Big)$$

$$\psi_i^n(v)=\rho_i^n\sqrt{T_i^n}\ \zeta\Big(\frac{(v-u_i^n)}{\sqrt{T_i^n}}\Big)$$

give us:

$$U_i^n=\int_{\Re}(\phi_i^n,v\phi_i^n,\frac{v^2}{2}\phi_i^n+\psi_i^n)\ dv$$

and

$$U_i^{n+1}=U_i^n-\frac{\Delta t}{\Delta x}(F_{i+1/2}^n-F_{i-1/2}^n)\ ,$$

where $F_{i+1/2}^n=F^+(U_i^n)+F^-(U_i^{n+1})$ (flux splitting), with:

$$F^+(U_i^n)=\int_{v\ge 0}v\,(\phi_i^n,v\phi_i^n,\frac{v^2}{2}\phi_i^n+\psi_i^n)\ dv$$

$$F^-(U_i^n)=\int_{v\le 0}v\,(\phi_i^n,v\phi_i^n,\frac{v^2}{2}\phi_i^n+\psi_i^n)\ dv$$

It can be verified that $F(U)=F^+(U)+F^-(U)$, which ensures the consistency.
If we consider the transport equations, we obtain that ϕ_i^{n+1} and ψ_i^{n+1} are positive under the condition $\sigma|v|\le 1$ for all v such that $\phi_i^n(v)>0$ and $\psi_i^n(v)>0$.
As $\phi_i^n(v)$ and $\psi_i^n(v)$ can be non zero only for $|v|<|u_i^n|+\sqrt{\beta T_i^n}$, we finally get:

Lemma 8 *Under the CFL condition* $(|u_i^n|+\sqrt{\beta T_i^n})\sigma\le 1$, *the kinetic scheme preserves the positivity of* ρ *and* T.

Having this wide variety of 1D positive schemes, we now wish to obtain positivity results for bidimensional problems. We derive in the following section a CFL condition ensuring that the 2D schemes based on the 1D positive schemes still preserve the positivity of ρ.

3.5 A CFL Condition to Preserve Positivity in 2D

We consider in this section a 1D positive scheme for the Euler equations, valid under the CFL condition:

$$\frac{\Delta t|V_{max}|}{\Delta x}\le\alpha_1 \tag{20}$$

and we derive a condition on the flux at interface $i+1/2$ for the positivity.
We consider a situation where the left border condition is a mirror state, that is to say that $\rho_{i-1}^n=\rho_i^n$, $u_{i-1}^n=-u_i^n$ and $e_{i-1}^n=e_i^n$.
The first component of the flux function $F_{i-1/2}^1$ should thus be zero. It is verified by the three positive schemes that we described in the previous sections.
For the Godunov scheme, we have $F_{i-1/2}^1=W_{RP}^2(0,U_{i-1}^n,U_i^n)=0$, for symmetry reasons. Likewise, for the HLLE scheme, cf. [8]

$$F_{i-1/2}^1\ =\ \frac{b_{i-1/2}^rF^1(U_i)-b_{i-1/2}^lF^1(U_{i-1})}{b_{i-1/2}^r-b_{i-1/2}^l}\ +\ \frac{b_{i-1/2}^r\ b_{i-1/2}^l}{b_{i-1/2}^r-b_{i-1/2}^l}(U_i^n-U_{i-1}^n)\ .$$

And $U_i^n = U_{i-1}^n = \rho_i^n$, $F^1(U_i) = u_i^n = -F^1(U_{i-1})$, $b_{i-1/2}^r = -b_{i-1/2}^l$ for symmetry reasons. Therefore, we get that $F_{i-1/2}^1 = 0$.
Finally, for the kinetic scheme, we get that $F^-(U_i^n) = -F^+(U_{i-1}^n)$ and once again $F_{i-1/2}^1 = 0$.

The discretized Equation (19) for the density can thus be written:

$$\rho_i^{n+1} = \rho_i^n - \frac{\Delta t}{\Delta x} F_{i+1/2}^1 \ .$$

We denote $F_{i+1/2}^1 = \phi_{i+1/2}$ and the positivity condition is now:

$$\frac{\Delta t \ \phi_{i+1/2}^+}{\rho_i^n \Delta x} \leq 1 \ .$$

We finally get:

Lemma 9 *A 1D scheme that can be written in the form (19) and that is positive under the CFL condition:*

$$\frac{\Delta t |V_{max}|}{\Delta x} \leq \alpha_1$$

satisfies the following property:

$$\frac{\alpha_1 \ \phi_{i+1/2}^+}{|V_{max}| \rho_i^n} \leq 1 \ . \tag{21}$$

Definition 1 : ρ-positive flux decomposition
More generally, considering a Riemann problem between two states U_R and U_L, $|V_{max}|$ being the maximum wave speed between these two states, we will say that a flux decomposition ϕ is ρ-positive if:

$$\frac{|V_{max}| \Delta t}{\Delta x} < \alpha \quad \textit{implies} \quad \frac{\Delta t \, \phi^+(U_L, U_R)}{\rho_L \Delta x} < 1 \ .$$

We will then get:

$$\frac{\alpha_1 \ \phi^+(U_L, U_R)}{|V_{max}| \rho_L} \leq 1 \ . \tag{22}$$

For bidimensional problems, a finite-volume discretization of the mass conservation gives:

$$a_i \rho_i^{n+1} = a_i \rho_i^n - \Delta t \sum_{j \in V(i)} \phi_{ij} \, l_{ij} \ , \tag{23}$$

where $l_{ij} = ||\vec{\eta_{ij}}|| = || \int_{C_i \cap C_j} \vec{\eta} \ ds||$.
ϕ_{ij} corresponds to a 1D flux between the states U_i^n and U_j^n. Therefore, using (22) we successively get:

$$\begin{aligned} \phi_{ij} &\leq \frac{|V_{max}| \rho_i^n}{\alpha_1} \\ \Delta t \sum_{j \in V(i)} \phi_{ij} l_{ij} &\leq \frac{|V_{max}| \rho_i^n \Delta t}{\alpha_1} \Big(\sum_{j \in V(i)} l_{ij} \Big) \end{aligned}$$

As in Section 2.3, we use the boundary measure $L_i = \left(\sum_{j \in V(i)} l_{ij} \right)$, and with (23), we finally get that ρ_i^{n+1} is positive provided that:

$$\frac{|V_{max}| \Delta t}{\alpha_1 (\frac{a_i}{L_i})} \leq 1 \ .$$

Lemma 10 *The 2D scheme built from a ρ-positive decomposition is ρ-positive under the CFL condition:*

$$\frac{|V_{max}|\Delta t}{(\frac{a_i}{L_i})} \leq \alpha_1 \ . \tag{24}$$

We now wish to derive high-order positive schemes in 2D.
We suppose that all the ρ_j^n are positive. The general form of the discrete equation giving ρ_i^{n+1} that we consider is now written:

$$\begin{aligned} a_i\rho_i^{n+1} &= a_i\rho_i^n - \Delta t \sum_{j\in V(i)} \phi_{ij}^{HO} l_{ij} \\ &= a_i\rho_i^n - \Delta t \sum_{j\in V(i)} \left(\frac{\phi_{ij}^{HO+} l_{ij}}{\rho_{ij}}\right)\rho_{ij} + \left(\frac{\phi_{ij}^{HO-} l_{ij}}{\rho_{ji}}\right)\rho_{ji} \ , \end{aligned} \tag{25}$$

where ϕ a ρ-positive flux decomposition and $\phi_{ij}^{HO} = \phi(U_{ij}, U_{ji})$. If ρ_{ij} and ρ_{ji} are positive, we can identify:

$$(\vec{V_{ij}}.\vec{\eta_{ij}})^+ = \frac{\phi_{ij}^{HO+} l_{ij}}{\rho_{ij}} \text{ and } (\vec{V_{ij}}.\vec{\eta_{ij}})^- = \frac{\phi_{ij}^{HO-} l_{ij}}{\rho_{ji}} \ ,$$

and Equation (25) is exactly under the form of Equation (12) in Section 2.3. The same argument will apply if we use the same reconstruction:

$$\begin{aligned} \rho_{ij} &= \rho_i + \tfrac{K^-}{2}\Big(\epsilon_{ri}(\rho_i - \rho_r) + \epsilon_{si}(\rho_i - \rho_s)\Big) &= \rho_i + \tfrac{K_1^0}{2}(\rho_j - \rho_i) \\ \rho_{ji} &= \rho_j - \tfrac{K_2^0}{2}(\rho_j - \rho_i) \, , \end{aligned}$$

with K^-, K_1^0, K_2^0, ϵ_{ri} and ϵ_{si} all positive.
First, as $K_1^0 \leq 2$ and $K_2^0 \leq 2$ we get from these equations that:

$$min(\rho_i, \ \rho_j) \leq \rho_{ij}, \ \rho_{ji} \leq max(\rho_i, \ \rho_j) \ ,$$

ρ_{ij} and ρ_{ji} are actually positive.
We can rewrite the discrete Equation (25) as follows:

$$\rho_i^{n+1} = \rho_i^n\left(1 - \frac{\Delta t}{a_i}\sum_{j\in V(i)}\left(\frac{\phi_{ij}^{HO+} l_{ij}}{\rho_{ij}}\right)(1 + K^- \frac{\epsilon_{ri}+\epsilon_{si}}{2}) + \frac{\Delta t}{a_i}\sum_{j\in V(i)}\left(-\frac{\phi_{ij}^{HO-} l_{ij}}{\rho_{ji}}\right)\frac{K_2^0}{2}\right) + \sum_{j\in V(i)} \alpha_j\rho_j^n$$

and, as in Section 2.3, the positivity of ρ is preserved provided that:

$$\frac{\Delta t}{a_i}\sum\left(\frac{\phi_{ij}^{HO+} l_{ij}}{\rho_{ij}}\right) \leq \frac{1}{1+M}, \tag{26}$$

with M a mesh charactersitic.
$\phi_{ij}^{HO} = \phi(U_{ij}, U_{ji})$ with ϕ a ρ-positive flux decomposition, and we get as in Lemma 10:

$$\frac{\alpha_1\phi_{ij}^{HO+}}{|V_{max}|\rho_{ij}} \leq 1 \tag{27}$$

$L_i = \sum_{j\in V(i)} l_{ij}$ and with (26) and (27) we finally get the following lemma:

Lemma 11 *The quasi third-order scheme introduced in Section 2.3, cf. Equations (13) and (14), based on a ρ-positive flux decomposition is ρ-positive under the CFL condition:*

$$\frac{\Delta t \ |V_{max}|}{(\frac{ai}{L_i})} \leq \frac{\alpha_1}{1+M} \ , \tag{28}$$

Remark 6

The same argument applies for higher-order scheme involving the same type of limiters, cf. [4].

4 Maximum Principle for the Mass Fractions in Multi-component Flows

We consider now a compressible multi-component flow. Larrouturou in [13] derived a scheme that preserves the maximum principle for the mass fractions for 1D first-order and second-order schemes and for 2D first-order schemes. Our purpose is to extend Larrouturou's result to 2D second-order schemes.

4.1 First-Order Scheme in 2D

First, we recall the two-component Euler equations in one dimension:

$$\frac{\partial U}{\partial t} + \frac{\partial F(U)}{\partial x} + \frac{\partial G(U)}{\partial y} = 0 \tag{29}$$

$$U = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ e \\ \rho Y \end{pmatrix} \qquad F(U) = \begin{pmatrix} \rho u \\ \rho u^2 + P \\ \rho u v \\ (e+P)u \\ \rho u Y \end{pmatrix} \qquad G(U) = \begin{pmatrix} \rho v \\ \rho u v \\ \rho v^2 + P \\ (e+P)v \\ \rho v Y \end{pmatrix} \tag{30}$$

where we use the notations given in Section 3, and where Y is the mass fraction of the first species. The presuure is given by:

$$P = (\gamma - 1)\left(e - \frac{1}{2}(u^2 + v^2)\right)$$

The first four equations are the classical Euler equations for the mixture, and the last one is a "species" equation. More generally, a convected variable is involved in this last equation, here the mass fraction, but it could be k or ϵ for a turbulent problem.
The explicit conservative discretization of the problem is given by:

$$a_i \, \frac{U_i^{n+1} - U_i^n}{\Delta t} = - \sum_{j \in V(i)} \Phi(U_i, U_j, e\vec{t}a_i j) = - \sum_{j \in V(i)} \Phi_{ij} l_{ij}. \tag{31}$$

Larrouturou's idea is to evaluate the first four components of the numerical flux with a classical Godunov-type scheme and the last component of the flux is defined as follows:

$$\Phi_{ij}^5 = \Phi_{ij}^{1+} Y_i^n + \Phi_{ij}^{1-} Y_j^n \tag{32}$$

With this construction and under a CFL-like condition, the scheme preserves the maximum principle for the mass fraction Y, cf. [13].
In his argument, Larrouturou needs to assume that the positivity of ρ is preserved. Here, we show the following lemma:

Lemma 12 *if we use a ρ-positive scheme to evaluate the first four components of the flux corresponding to the mixture flow, no extra CFL condition (than the one for the ρ-positivity) is actually needed to ensure the preservation of the maximum principle for the mass fraction.*

Proof: We note:

$$\phi_{ij} = \Phi_{ij}^1 \,,$$

and we get the discretized equations for ρ and ρY under the following form:

$$\left\{ \begin{array}{rcl} \rho_i^{n+1} & = & \rho_i^n - \Delta t \, \sum_{j \in V(i)} \phi_{ij} \left(\frac{l_{ij}}{a_i}\right) \\ \rho_i^{n+1} Y_i^{n+1} & = & \rho_i^n Y_i^n - \Delta t \, \sum_{j \in V(i)} (\phi_{ij}^+ Y_i + \phi_{ij}^- Y_j) \left(\frac{l_{ij}}{a_i}\right) \end{array} \right.$$

We know that ρ_i^{n+1} is positive. Therefore we can rewrite the last equation under the form:

$$Y_i^{n+1} = \left(\frac{\rho_i^n - \Delta t \sum_{j\in V(i)} \phi_{ij}^+ (\frac{l_{ij}}{a_i})}{\rho_i^n - \Delta t \ \sum_{j\in V(i)} \phi_{ij} (\frac{l_{ij}}{a_i})} \right) Y_i^n + \sum_{j\in V(i)} \left(\frac{(-\phi_{ij}^-)\Delta t (\frac{l_{ij}}{a_i})}{\rho_i^n - \Delta t \ \sum_{j\in V(i)} \phi_{ij} (\frac{l_{ij}}{a_i})} \right) Y_j^n \ . \tag{33}$$

As:

$$\rho_i^n - \Delta t \sum_{j\in V(i)} \phi_{ij} \left(\frac{l_{ij}}{a_i} \right) = \rho_i^{n+1} > 0 \ ,$$

and as ϕ is a ρ-positive decomposition, with the positivity condition (22) and the CFL condition (24), we get:

$$\rho_i^n - \Delta t \sum_{j\in V(i)} \phi_{ij}^+ \left(\frac{l_{ij}}{a_i} \right) > 0$$

we can rewrite (33) in the form:

$$Y_i^{n+1} = \alpha_i Y_i^n + \sum_{j\in V(i)} \alpha_j Y_j^n$$

where all the α_k are in $[0;1]$ and $\sum_k \alpha_k = 1$
Y_i^{n+1} is a convex combination of the Y_k^n,therefore:

$$\min_{j\in V(i),\ j=i} Y_j^n \leq Y_i^{n+1} \leq \max_{j\in V(i),\ j=i} Y_j^n \ ,$$

and the maximum principle is thus preserved. We can note that only the CFL condition used for the ρ-positivity is needed. □

4.2 A High-Order Scheme in 2D

We now wish to obtain the maximum principle for higher-order schemes. For this purpose, we use a high-order solver for the Euler equations that still preserves the positivity of ρ, cf. Section 3.5, and the discretized equation for ρ and ρY are now written:

$$\left\{ \begin{array}{rcl} \rho_i^{n+1} & = & \rho_i^n - \Delta t \ \sum_{j\in V(i)} \phi_{ij} (\frac{l_{ij}}{a_i}) \\ \rho_i^{n+1} Y_i^{n+1} & = & \rho_i^n Y_i^n - \Delta t \ \sum_{j\in V(i)} (\phi_{ij}^+ Y_{ij} + \phi_{ij}^- Y_{ji}) \left(\frac{l_{ij}}{a_i} \right) \end{array} \right.$$

We use here the quasi third-order reconstruction introduced in Section 2.3:

$$\left\{ \begin{array}{rcl} Y_{ij} & = & Y_i + \frac{K^-}{2} \Big(\epsilon_{si} (Y_i - Y_s) + \epsilon_{ri} (Y_i - Y_s) \Big) \\ \\ Y_{ji} & = & Y_j - \frac{K_2^0}{2} (Y_j - Y_i) \end{array} \right.$$

And we get:

$$\begin{array}{rcl} \rho_i^{n+1} Y_i^{n+1} & = & Y_i^n \left(\rho_i^n - \Delta t \displaystyle\sum_{j\in V(i)} \phi_{ij}^+ \Big(1 + \frac{K^-}{2} (\epsilon_s + \epsilon_r) \Big) \Big(\frac{l_{ij}}{a_i} \Big) + \Delta t \sum_{j\in V(i)} (-\phi_{ij}^-) \frac{K_2^0}{2} \Big(\frac{l_{ij}}{a_i} \Big) \right) \\ & & + \Delta t \displaystyle\sum_{j\in V(i)} \phi_{ij}^+ \Big(\frac{l_{ij}}{a_i} \Big) \Big(\frac{K^- \epsilon_{si}}{2} Y_s^n + \frac{K^- \epsilon_{ri}}{2} Y_r^n \Big) \\ & & + \Delta t \displaystyle\sum_{j\in V(i)} (-\phi_{ij}^-) (1 - \frac{K_2^0}{2}) \left(\frac{l_{ij}}{a_i} \right) Y_j^n \end{array}$$

Here, vertices s and r depend on vertex j, but we have chosen not to complicate the notations. Under the CFL condition ensuring the positivity of ρ, cf. Equation (28), all the coefficients of this Y-decomposition are non-negative and their sum is equal to ρ_i^{n+1}. Therefore, Y_i^{n+1} can be written as a convex linear combination of Y_j^n, $j \in V(i)$ or $j = i$, and the maximum principle is thus preserved with no extra CFL condition.

5 Conclusion

This paper proposes a synthesis of many contributions to Godunov-type finite-volume methods. We have examined the question of positivity for the scalar advection equation and the Euler equations, particularly for 2D triangulations and explicit time discretization. The proposed limited interpolation gives us a quasi third-order, positive scheme for the scalar advection equation. Combined with a ρ-positive flux decomposition (for example the HLLE or Perthame ones), it also gives a quasi third-order explicit scheme that preserves the positivity of density for the Euler equations.

We have also discussed the importance of the CFL condition for the positivity and the danger of an irregular mesh when the interpolation is made with the upstream and downstream triangles.

Finally, for bidimensional multi-component flows, we have extended Larrouturou's result by obtaining thanks to our limiter a quasi third-order scheme that preserves the maximum principle for mass fractions.

As a result, the ρ-positivity of practical (second-order accurate) software for compressible Euler flow simulation on unstructured mesh is now well established and robustness of $k-\epsilon$ or multi-component flow calculations is also improved although not completely solved. Moreover, the 3D extension follows without conceptual difficulty.

Nevertheless, some issues remain unsolved. Firstly, the positivity of temperature for high-order schemes does not come easily yet, but the solution might result from Perthame's works, cf. [14]. Another concern is the implicit time discretization, we are preparing a second paper analysing the case of implicit positive schemes.

Finally, besides our edge-wise finite-volume scheme, some other multidimensional methods could be examined for the ρ-positivity issue. Barth proposed in [2] bidimensional reconstruction and limitation that could allow us to enforce positivity. Moreover, the MDHR method developed by Sidilkover in [16] and Deconinck *et al.* in [6] are genuinely bidimensional extensions of the Roe scheme and thus offer a lot of new possibilities for investigation.

References

[1] K. Baba and M. Tabata. On a conservative upwind finite element scheme for convective diffusion equations. *R.A.I.R.O Numer. Anal. 15*, 3-25 (1981).

[2] T.J. Barth. Aspects of Unstructured Grids and Finite Volume Solvers for the Euler and Navier-Stokes Equations. *Von Karman Institute Lecture Notes*, 1994.

[3] J.P. Boris and D.L. Book. Flux corrected transport, 1 SHASTA, a fluid transport algorithm that works. *Journal of Computational Physics*, 11, 38-69, 1973.

[4] C. Debiez, A. Dervieux, and P. Arminjon. Mixed-Element-Volume: Bridging Finite Elements and Positive Finite Volumes; some Accuracy Issues. *Proceedings of the CERCA, Conference on Numerical Methods for the Euler and Navier-Stokes Equations.*, Montreal, 14-16 Septembre 1995.

[5] C. Debiez, A. Dervieux, K. Mer, and B. Nkonga. Computation of Unsteady Flows with Mixed Finite Volume/Finite Element Upwind Methods. *Proceedings, IX International Conference on Finite Elements in Fluids, New Trends and Applications.*, Venise, 15-21 Octobre 1995.

[6] H. Deconinck, P.L. Roe, and R. Struijs. A Multidimensional Generalization of Roe's Flux Difference Splitter for the Euler Equations. *Computers Fluids*, Vol. 22. , No 23, pp 215-222 (1993).

[7] B. Einfeldt. On Godunov-type Methods for Gas Dynamics. *SIAM J. Numer. Anal.*, 25, (April 1988).

[8] B. Einfeldt, C.D Munz, P.L. Roe, and B. Sjogreen. On Godunov-type Methods near Low Densities. *Journal of Computational Physics*, 92, 273-295 (1991).

[9] L. Fezoui and A. Dervieux. Finite Element Non Oscillatory Schemes for Compressible Flows. *Proceedings, 8th France-USSR-Italy Joint Symposium on Computational Mathematics and Applications*, Pavia, October 2-6 1989.

[10] A. Harten, P.D Lax, and B. Van Leer. On Upstream Differencing and godunov-type Schemes for Hyperbolic Conservation Laws. *SIAM Review*, 25, 35-61, 1983.

[11] A. Jameson. Artificial Diffusion, Upwind Biasing, Limiters and their Effect on Accuracy and Multigrid Convergence in Transonic and Hypersonic Flows. *AIAA paper 3359*, (1993).

[12] T. Jongen and Y.P. Marx. Design of an Unconditionnaly Stable, Positive Scheme for the $k-\epsilon$ and Two Layer Turbulence Model. *Computers and Fluids*, Vol. 26. No. 5. pp. 469-487 (1997).

[13] B. Larrouturou. How to Preserve the Mass Fraction Positivity when Computing Compressible Multi-component Flows. *Journal of Computational Physics*, 95, 59-84 (1991).

[14] B. Perthame and B. Khobalate. Maximum Principle on the Entropy and Minimal Limitations for Kinetic Scheme. *Rapports de Recherche INRIA*, 1628, (1992).

[15] C.W. Shu and Osher S. Efficient Implementation of Essential Non-oscillatory Shock Capturing Schemes. *Journal of Computational Physics*, 77, 439-471 (1988).

[16] D. Sidilkover. A Genuinely Multidimensional Upwind Scheme and Efficient Multigird Solver for the Compressible Euler Equations. *ICASE Report No. 94-84*, (1994).

[17] B. Van Leer. Towards the Ultimate Conservative Difference Scheme V: A Second Order Sequel to Godunov's Method. *Journal of Computational Physics*, 32, 101-136 (1979).

Unité de recherche INRIA Sophia Antipolis
2004, route des Lucioles - B.P. 93 - 06902 Sophia Antipolis Cedex (France)

Unité de recherche INRIA Lorraine : Technopôle de Nancy-Brabois - Campus scientifique
615, rue du Jardin Botanique - B.P. 101 - 54602 Villers lès Nancy Cedex (France)
Unité de recherche INRIA Rennes : IRISA, Campus universitaire de Beaulieu - 35042 Rennes Cedex (France)
Unité de recherche INRIA Rhône-Alpes : 655, avenue de l'Europe - 38330 Montbonnot St Martin (France)
Unité de recherche INRIA Rocquencourt : Domaine de Voluceau - Rocquencourt - B.P. 105 - 78153 Le Chesnay Cedex (France)

Éditeur
INRIA - Domaine de Voluceau - Rocquencourt, B.P. 105 - 78153 Le Chesnay Cedex (France)
http://www.inria.fr
ISSN 0249-6399